Meyer, Spaeth, and Scheffler Respond: Kaufmann<sup>1</sup> interprets the experimental magnetic circular dichroism (MCD) of the As-antisite defect in GaAs<sup>2</sup> as an optically excited transition of a valence band electron into the  $D^+$  state of the defect,  $D^+ \rightarrow D^0 + h_{\nu}$ . The presentation and justification of this interpretation are, however, erroneous:

(1) Apparently there is no dispute that the symmetry of the isolated As antisite is tetrahedral and that the deep-level wave function belongs to the  $A_1$  representation.<sup>1-3</sup> This has been recently confirmed by detailed electron-nuclear double-resonance experiments,<sup>4</sup> which were also performed on the same sample as our original MCD measurements. Therefore, the possible final states of optically detected transitions, which involve the deep level, belong to the  $T_2$ representation. If the spin-orbit interaction is taken into account, each  $T_2$  level splits into two levels and an absorption experiment detects each  $A_1$ - $T_2$  transition as two lines. In an MCD experiment, which measures the difference of the absorption of left and right circularly polarized light, these two absorption peaks occur as one peak with positive and one peak with negative amplitude (i.e., derivativelike structure). Therefore, the MCD of Ref. 2 must be due to a superposition of derivativelike structures. This is what was done in Ref. 2 (see the fit in Fig. 2 of Ref. 2). The occurrence of one derivative- and one bell-shaped structure, as proposed in Ref 1, is only possible for a distorted defect.

(2) If an optical excitation in a system of  $T_d$  symmetry involves transitions between Bloch states and a deep  $A_1$  level, a proper linear combination of these Bloch states must be chosen, which belongs to the  $T_2$  representation. This is apparently overlooked in the third paragraph of Ref. 1.

(3) In contradiction to Kaufmann, we emphasize that theoretical and experiment evidence for two or more excited  $T_2$  states is well known for most semiconductors: In our original paper,<sup>2</sup> we already mentioned the theoretical work on the P antisite in GaP.<sup>5</sup> This theoretically predicted multiple-peak structure of the conduction band  $T_2$  density of states was indeed observed in recent MCD measurements.<sup>6</sup> Concerning the self-consistent calculations of Bachelet, Schlüter, and Baraff,<sup>7</sup> which are cited by Kaufmann to support his doubts, we note the following: (i) These calculations do not include spin-orbit splitting, which is the fundamental mechanism which makes the MCD work. (ii) The figures in this paper<sup>7</sup> refer to the *neutral* state of the As antisite, not to the paramagnetic charge state  $D^+$  relevant for the MCD. For the  $D^+$  center a Coulombic tail is present, which (among other effects) pulls states down also from the conduction band at X. In this respect, the situation in GaAs is very similar to that of Si (if one just neglects the very low GaAs conduction band density of states at  $\Gamma$ ). For excitation of  $D^+$  states of deep donors in Si it is well known

that there is more than one excited  $T_2$  state (see, e.g., Janzen *et al.*<sup>8</sup>)

(4) The model in Ref. 1 requires that the electronic transitions are well localized in k space, i.e., that only Bloch states close to  $\Gamma$  are important. This localization in k space conflicts with the established electronic properties of the As antisite. We emphasize that the As antisite is a deep defect, which implies that the deep-level wave function is well delocalized in k space. This aspect is confirmed by recent electron-nuclear double-resonance investigations<sup>4, 6</sup> and by the theoretical results,<sup>7</sup> which also show that the As-antisite level in k space and the fact that the defect-induced  $T_2$  density of states at the top of the valence band is nearly zero rule against Kaufmann's model.

Because of the space limitations, only a few (not all) problems of Kaufmann's arguments could be discussed above. A more complete discussion will be provided upon request.<sup>9</sup> All currently known experimental and theoretical results support our model presented in Ref. 2. We therefore repeat the conclusion based on this model, namely, that the *EL*2 center in GaAs is not due to an isolated As antisite. We also note that recently this conclusion has been confirmed by other investigations.<sup>4, 6, 10</sup>

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<sup>1</sup>U. Kaufmann, preceding Comment [Phys. Rev. Lett. 54, 1332 (1985)].

 $^{2}B.$  K. Meyer, J.-M. Spaeth, and M. Scheffler, Phys. Rev. Lett. **52**, 851 (1984).

<sup>3</sup>R. Wörner, U. Kaufmann, and J. Schneider, Appl. Phys. Lett. **40**, 141 (1982).

<sup>4</sup>D. M. Hofmann, B. K. Meyer, F. Lohse, and J.-M. Spaeth, Phys. Rev. Lett. **53**, 1187 (1984).

 $^{5}$ M. Scheffler, J. Bernholc, N. O. Lipari, and S. T. Pantelides, Phys. Rev. B **29**, 3269 (1984).

<sup>6</sup>B. K. Meyer and J.-M. Spaeth, to be published.

<sup>7</sup>G. B. Bachelet, M. Schlüter, and G. A. Baraff, Phys. Rev. B 27, 2545 (1983).

<sup>8</sup>E. Janzen, R. Stedman, G. Grossmann, and H. G. Grimmeiss, Phys. Rev. B 29, 1907 (1984).

<sup>9</sup>B. K. Meyer, J.-M. Spaeth, and M. Scheffler, unpublished.

<sup>10</sup>M. Taniguchi and T. Ikoma, Appl. Phys. Lett. **45**, 69 (1984); J. Lagowski and H. C. Gatos, J. Electron. Mater. **14A**, 73 (1985); M. Scheffler *et al.*, J. Electron. Mater. **14A**, 45 (1985); B. K. Meyer *et al.*, J. Electron. Mater. **14A**, 921 (1985); G. B. Bachelet and M. Scheffler, in *Proceedings of the Seventeenth International Conference on Physics of Semiconductors, San Francisco, 1984* (Springer, New York, 1985).